Optoelectronic Materials and Devices
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Module - 01
Electronic Structure of Materials
Lecture - 04
Crystal Structure, Reciprocal Lattice I

So, welcome for… Welcome to lecture four. Let me just take few moments, so that things do not appear disjointed. Ultimately, I will tell you, what we are trying to do. We are trying to get to understand real E versus k diagram. And, you will notice that, I have been stressing, this conductivity business – how conduction happens, etcetera; you think a sort of this little bit side business, but of course important. But, all along in trying to explain that, we are developing some ideas. I have shown you k vector – origin of k vector in free electron theory, which is a wave vector. I have shown you that, this k vector also means momentum. We have energy versus k relationship. We want to plot this E-k diagram.

Eventually, as we go along, I will show you that, E-k diagram contains all the information you require for electron dynamics; it tells us the properties of materials; it tells us whether it is a good optical material, which is what the subject of this course is or it is not. How things become the semiconductors, etcetera, etcetera – are all corrected to this, which we will be covering in this course. So, ultimately or at this point of time, the goal is to make sure that, you understand what E-k diagram is. When I show you the real E-k diagram, it will be complicated messy diagram. In next, therefore, two-three lectures or four lectures, what I am going to do is slowly build up the case, which explains what is the justification for drawing the real E-k diagram, which I will be showing you little bit later. Interim, which I am trying to buildup (( )) conductivity – understanding of why we are introducing each idea.

We have gone up to free electron theory and we have shown you that, free electron theory does not explain everything, because it does not have an idea of lattice underneath. So, what we have to do is now, explain lattice; given a lattice, I will show you the… I will also explain reciprocal lattice and its sole purpose would or main purpose would be that, you will see that, this k vector lies in reciprocal space; its dimension is inverse of length. So, imagine in a space in which all the scales are in inverse of length. So, reciprocal lattice vectors would lie in that space and they might play an important role. And, that role I will show you the role reciprocal lattice vectors; not the reciprocal lattice by itself, but reciprocal lattice vectors, which will have, will be useful in constructing the E-k diagram. That is why we want to introduce these two ideas at this point of time. Eventually, what I will do is…

And, remember in free electron theory, we also did not put any potential; we said it is free electron; that means it does not see other ions; it does not see any potential because of that. We made the v term equal to 0. But, eventually, really that is not correct, because there is an underlying lattice; we will should have a potential; and, that potential should be periodic having periodicity of the lattice. We will have to introduce that. And, when we introduce that, some remarkable things will happen; and, you would be able to understand why some materials are metal, why some materials are insulator and why some materials are semiconductor; which free electron theory cannot do. Remember – it is really good for only metals.

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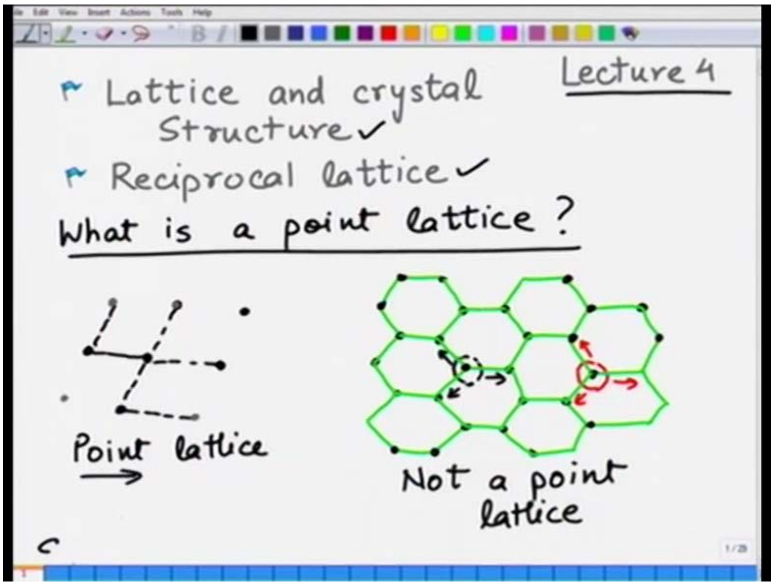

But, because metals is where there is a hope for electron to be free electron. Other places, it will not be a free electron; and, there you will start seeing the semiconducting behavior also. So, that is the reason we are trying to move in this direction. And, this lattice and crystal structure and reciprocal lattice is a review. I am just going to review, so that I take along all the students. But, I expect most of you to have seen this before. Therefore, I will go little fast and only pick only in the relevant portion. So, this is a review.

So, this lecture number four is a review lecture on lattice and crystal structure and reciprocal lattice. I will just take the fundamentals here and not great details in here. So, more this will be a dialogue; this will be more of a question asked, answer given; question asked, answer given. That is how we will produce… That is how we will move along on these two topics today. So, let us do that. So, first question asked – what is a point lattice? That is the first question we are going to ask. What is a point lattice? Point lattice… Remember, first, what is a lattice or point lattice? First of all, remember lattice is not crystal structure; lattice is imaginary array of points. It is just imaginary array of points. You think of points arrange in space; you think of, not actually put something there. But, you just think of them as some points in space. Let me give you an example.

Let us say here are some points. Let me draw these points somewhere here like this, like this, like this, like this, like this, etcetera. We draw something like this. What do you see? What you see is that, if each point; and, if you take any point and that point looks identical; if I take this point and I stand here and look in particular direction; and then, I move out and I see the environment – how the environment looks like. If you go to another point – let us say this point and look in the same direction as I am looking from here; and, I find exactly same environment, same arrangement of points around here; that means each point in this imaginary point is a distribution point; any direction you look at on any point; you look at particular direction, not that you can…

In each direction, the view is same. In each direction, the view may be different. But, if you pick a direction, then you stand on any point, you will see the same view. That arrangement of points looks the same. That is really the definition of point lattice. So, this is an example of point lattice; where, if you stand here, then you see something is affect… You can see this is the orientation. If you stand here, you see the same orientation. If you stand here, you see the same orientation. You see the same orientation at any of these points. You see the same arrangement of points. If you see here, you see a point here. If you stand here, you see the corresponding point here. If you see here, you see corresponding similar point here. If you stand here, then you see a corresponding similar point right here; from here to here; from here to here or from here to here. You see some points are appear… They are identical points. The orientations are identical.

Example – a counter example may be arrangement of points, which is something like this. Let me see if I can draw a nice picture. I will attempt to first draw some pictures, not the points. I will draw some pictures; just hold on for a minute with me; and then, we will see… I will give you example, where which will not be a point lattice. Now, I think you can safely assume what I am trying to draw and hence continuously imagine this; and, think of these as the points – these imaginary array of points. So, remember, not all regular arrangement lead to point lattice. That example you can see from here; it is a nice regular arrangement of points, which you can see. This is a beautiful arrangement. But, notice that, if you pick this particular location; if you see, then you see a point in this direction; not atom, a point; a point in this direction, you see a point this direction.

But, if you stand somewhere else, another point; let us say you stand at this point; what do you see? In this case, there is a lattice point in this direction; there is lattice point in this direction. Clearly, the red type of lattice point – this red lattice point is quite different; has a different environment from the lattice point, which is black in color. So, clearly, you can see that, this cannot be a point lattice though it is a regular arrangement of points. So, that is one thing about I want to tell you. Then, what… So, point lattice – this is a point lattice; not a point lattice. So, now, let us look at what are the symmetry elements, which are underlying these point lattices.

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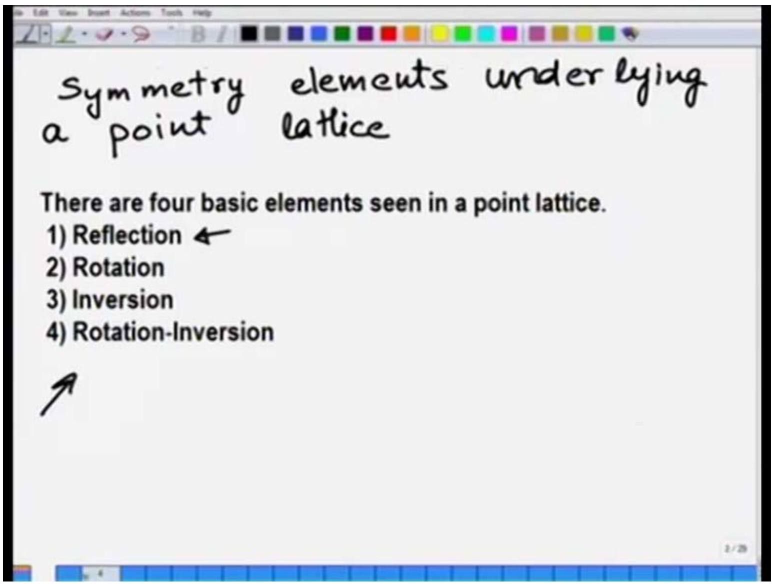

So, let us talk about symmetry elements underlying a point lattice. There are four basic symmetry elements that can be seen in a point lattice. One is of course this reflection; that means if you have… Let us say…

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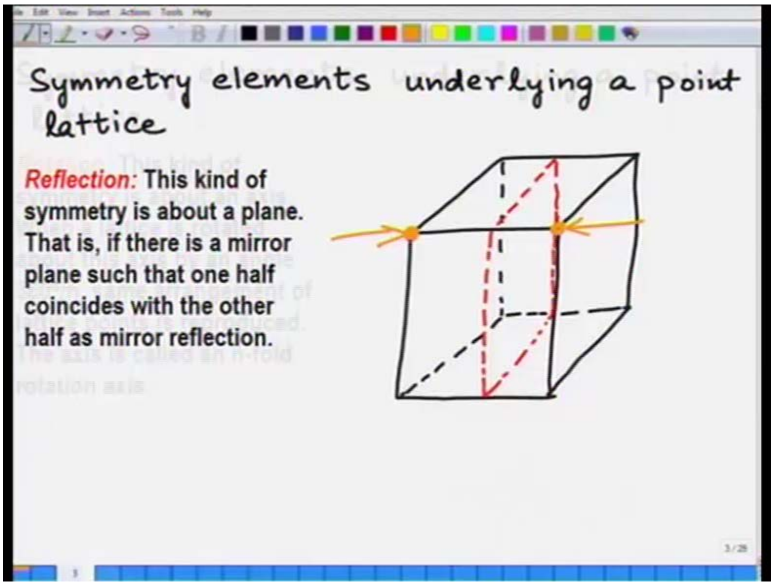

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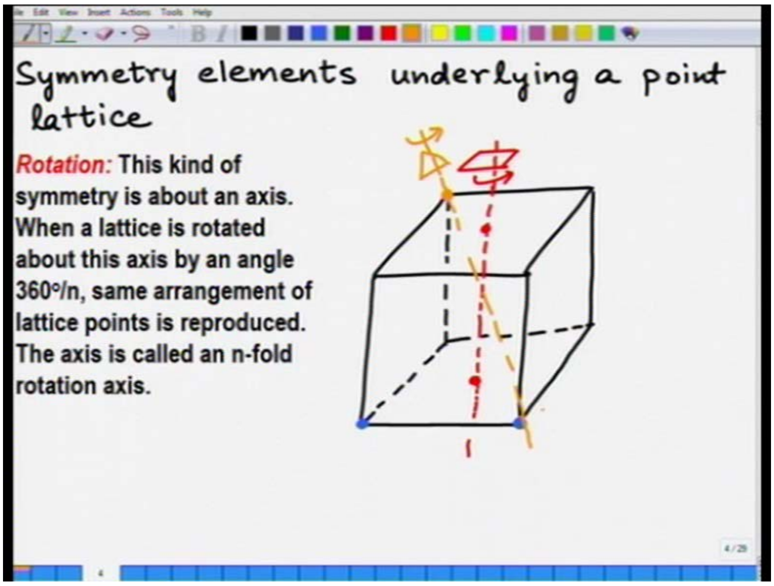

Let us do an example. Let us say something like this. Imagine this lattice. And, in this, you imagine a plane, which is looking something like this; imagine this plane; imagine this plane; about this plane, you can see that this point… About this plane, if you reflect this point, there is a lattice point. This kind of symmetry is about a plane; that is, if this is a mirror plane; that there is a mirror plane… So, I have drawn a red mirror plane such that one half on sides with the other half as mirror reflection. So, if every point, which appears on this side, let us say, this one – this point right here. If there is a mirror image of that always on the other side, then this is a reflection symmetry.

Similarly, we can think of this rotation symmetry. This kind of symmetry is about an axis. So, let us try to draw an axis and show you, in a cube, what this would be. Let us say that, we draw similarly, a cube again. This is a cube. Let us look at some axes in this. Let us imagine an axis, which runs like this. Right through the center, it runs like this. This is the axis. Imagine this axis right going through the center here and here. What do you see? You see a 4-fold axis. If you rotate this 90 degrees; if you (( )) 90 degrees, you will find that… If you rotate 90 degrees, then you will find that this point reaches this point. 90 degree – as you rotate 90 degree, the lattice looks the same. That is the rotation symmetry. Similarly, you can see a 3-fold rotation axis. If you wish, I can show you a 3-fold rotation axis all along the body diagonal.

If you look at this, take this point and this point. Along these points, if I draw a body diagonal like this, like this; and, you notice the tri rotating about this. This is a 3-fold. If you rotate it around it, you will see a 3-fold rotation axis; that means if you rotate it by 120 degrees, then you will generate basically the same structure essentially. So, this is a… If you… Therefore, it is called an n-fold axis or 3-fold axis and a 4-fold axis I have shown you. So, there could be a 2-fold axis; there could be 3-fold axis; there could be 4-fold axis; there could be 6-fold axis. But, there cannot be a 5-fold axis; think about that. Cossie crystal (( )) you have to think about.

Then, another kind of symmetry element is inversion. That is a point, is an inversion center. If every point on the lattice reproduces another lattice point equidistant from the inversion center on a line joining these two lattice points and also passing through the inversion center. So, you imagine like this. Instead of a mirror plane, it is a mirror coin. So, if every… If I am standing there in the center of the room; I look at one of the corners. And, if I reflect about this point; perpendicular to this, if I reflect… Or, rather I should say if I join these two points and continue the same distance in the other direction, then I will generate another point if I do final lattice point there. And, this happens for all the points, then it is an inversion center.

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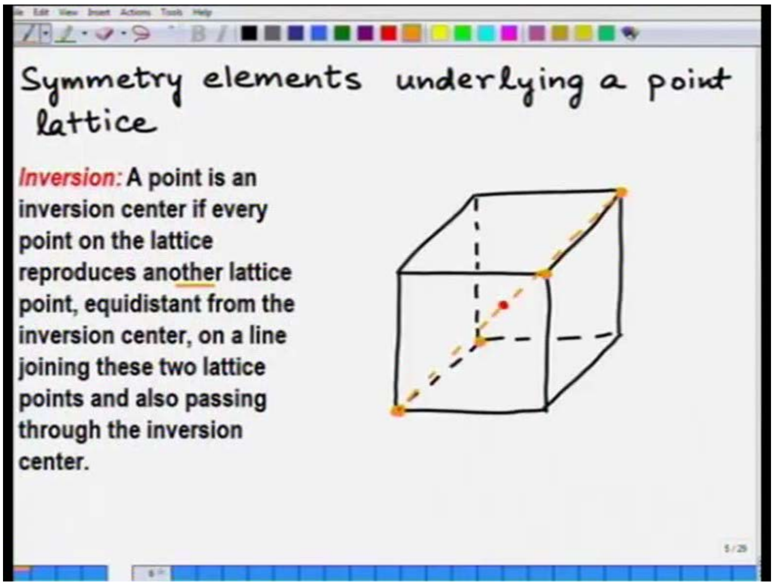

For example, let us draw one; again a cube and show through a cube, that inversion center in it. So, this is a cube I am drawing here. And, let us say if you put an inversion center right in the center of it, then you imagine that, I have a lattice point here. Then, whatever the distance I start joining these two points, I join these two points; and, I continue on this point an equal amount of distance, what I have just drawn. And then, if I do that and I find that I land up on another lattice position. And, that should happen for all the points. A point is an inversion center; every point on the lattice produces another lattice point. So, every point should be able to do that.

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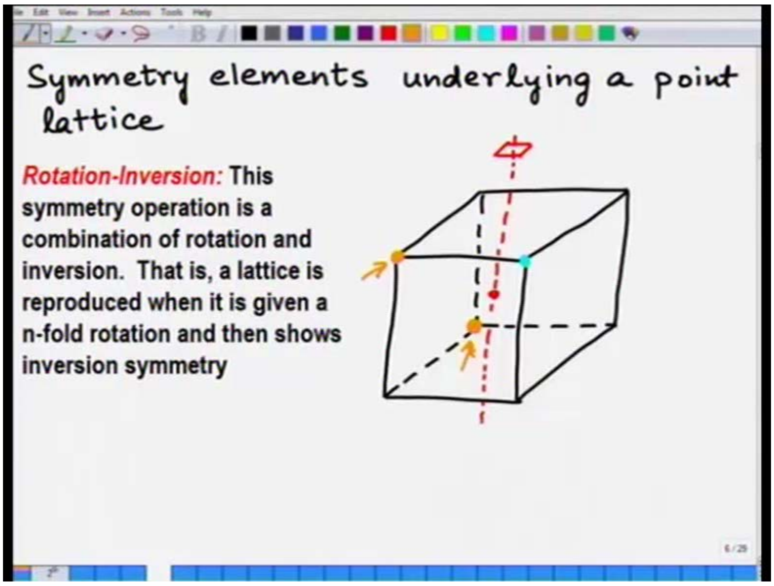

So, corresponding to this point, I will get another point here; corresponding to this point, I will get another point here, so on and so forth. So, this structure has an inversion symmetry. There is a point of inversion symmetry – inversion center in there. Rotation-inversion of same idea; essentially, it is a combination of rotation-inversion symmetry. This symmetry operation is a combination of rotation; that is, lattice is reproduced. If you give an n-fold rotation; whatever the rotation axis is – n fold rotation axis is, if you give rotation, it may not match at this stage. But, then there should be also inversion symmetry. And then, if you use inversion symmetry, then you will be able to generate a lattice. Example… Maybe I draw another example here through a cube for this case. So, this is this case; this is this case; this is this case. So, I draw another case – another thing right here. I do not know how good this drawing will turn out to be, but nonetheless, an attempt.

A cube for example, let us say a center right here. Here is a center. And, let us draw a… Remember the 4-fold rotation axis – a 4-fold rotation axis. And, this is also an inversion center. So, this is an inversion center and this is a 4-fold rotation axis. So, let us trace a point. What happens? Let us say that, I have point right here. So, I have a point here. Now, what we want to do? That we want to produce an n-fold rotation; so, 4-fold rotation we are going to do this about this axis. About this axis, when I do a 4-fold rotation, and I go rotation like this; 90 degrees I do. So, then where do I reach? Let me show you (( )) this color. So, we reach here. We reach here with… I reach here. This may be lattice point, this may not be lattice point; does not matter. But, after that, we do an inversion symmetry and then I reproduce the… About this point, inversion symmetry; then, I have reached this point right here. Now, you see what this says that is that, if you have a lattice point here, then a system if it has rotation inversion symmetry; then, you would have a lattice point here also and here also. That is the rotation-inversion symmetry operation as far as this is concerned. So, these are the point lattice.

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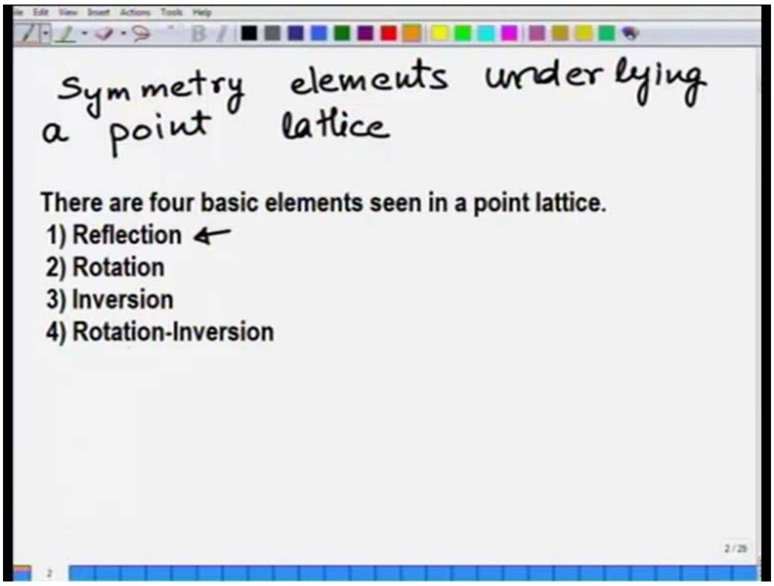

Underlying these point lattices are these therefore, symmetry elements.

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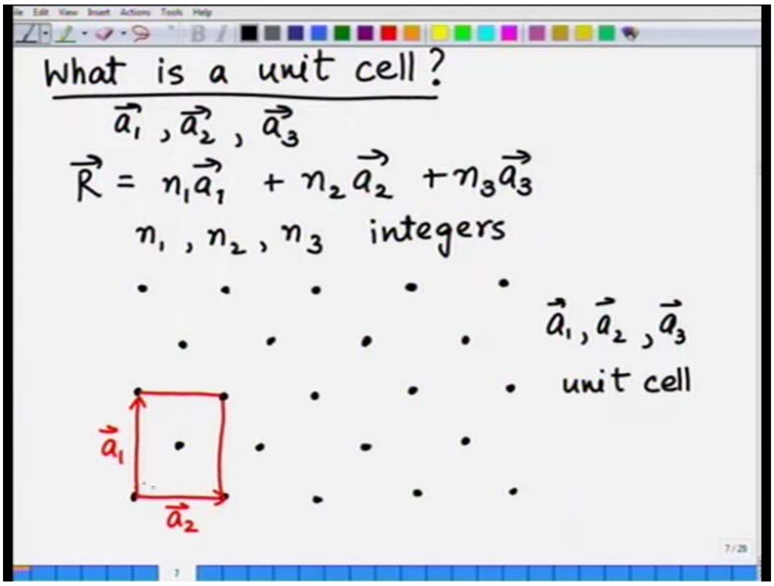

With these symmetry elements, now, let me define… Now, define one more thing before I… Second question is – what is a unit cell? Third question is what is a unit cell? What is a unit cell? So, now, we know that point lattice is a periodic lattice, the underlying symmetry elements. So, based on periodicity of the lattice, if you choose three vectors – non collinear vectors; then, in that case, not all in same plane. Then, I can describe those three lattice vectors by a 1, a 2 and a 3 as three vectors. Sometimes use an a, b, c; does not matter. a 1, a 2, a 3 are the three vectors. Then, I should be able to find position vectors; I should be able to position vectors of the point by R vector called n 1 a 1 plus n 2 a 2 plus n 3 a 3; that means I should be able to reproduce all the points by taking n 1, n 2 integers – n 1, n 2, n 3 integers. These are integers. So, I can take this and I should able to get to another point. This is one way to look at it.

Second thing is… Other way to look at it is that, a 1, a 2, a 3 – since they are three non-collinear vectors, they are not… Therefore, they will construct a volume. Whatever the volume is, if you translate this by distances a 1, a 2 and a 3, then you should be able to fill up the complete space generating those lattice points. These are two ways you can think of unit cells. So, there is a requirement of translation; that means you translate… I will give you a two-dimensional example that will make things little bit clear. For example, let us say I have something – a two-dimensional lattice; and, you imagine this in three dimension, something like this. In fact, let me make it little bit more complicated. Then, I am drawing here; let us say like this. So, some something like this.

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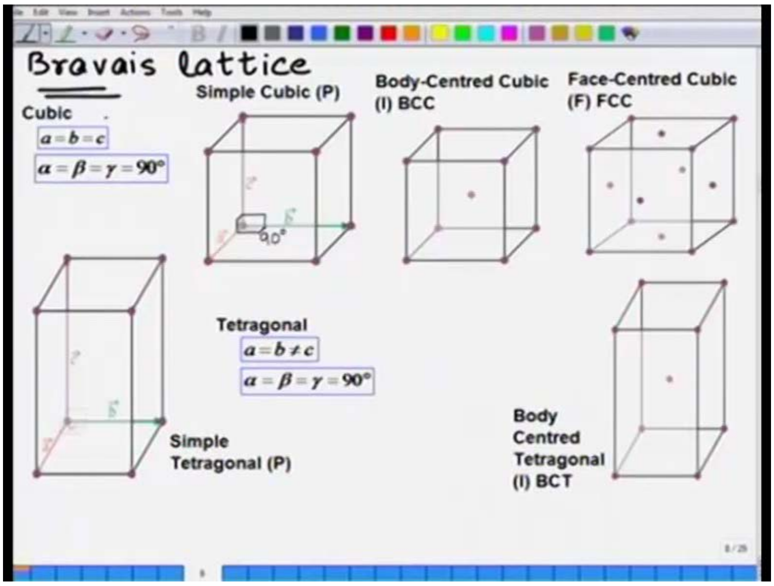

Suppose this is a lattice; I choose this to be… Or, I use different color here. So, let us say this is what I choose as the unit cell. This is a 1 vector; this is a 2 vector let us say. This is a 1 vector and a 2 vector right here; like this here. So, a 1, a 2 vector define this area. Now, you notice that, if I move this whatever area is constituted by a 1, a 2, we keep moving; we can generate all these lattice points. That is what is implied by a unit cell.

So, this is a good unit cell now. So, three vectors: a 1, a 2, a 3. So, a 1, a 2, a 3 define a unit cell. They define a unit cell. They are not necessarily the smallest volume, which we will see. By changing the angles or distances in size of magnitude of a 1, a 2, a 3 or the angles between them, there are seven types of as (( )) And, this is something you know.

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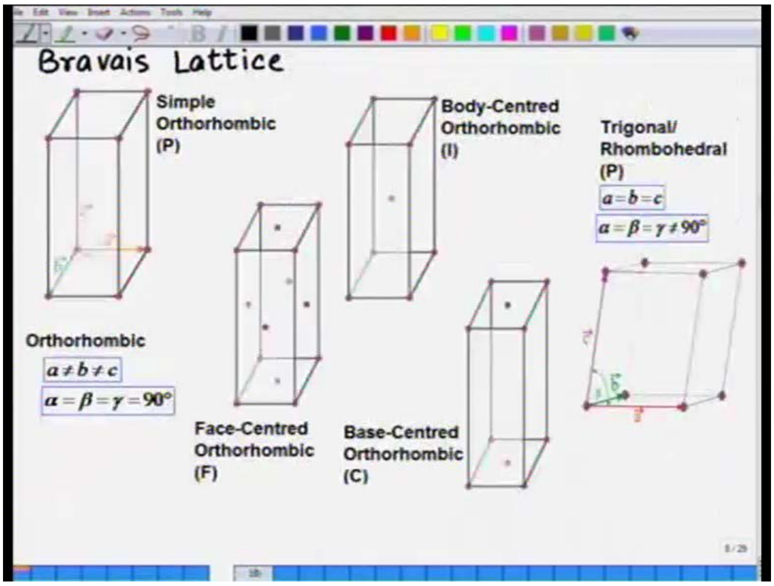

These are seven types of unit cells, are possible: the cubic, the tetragonal, the orthorhombic, the rhombohedral…

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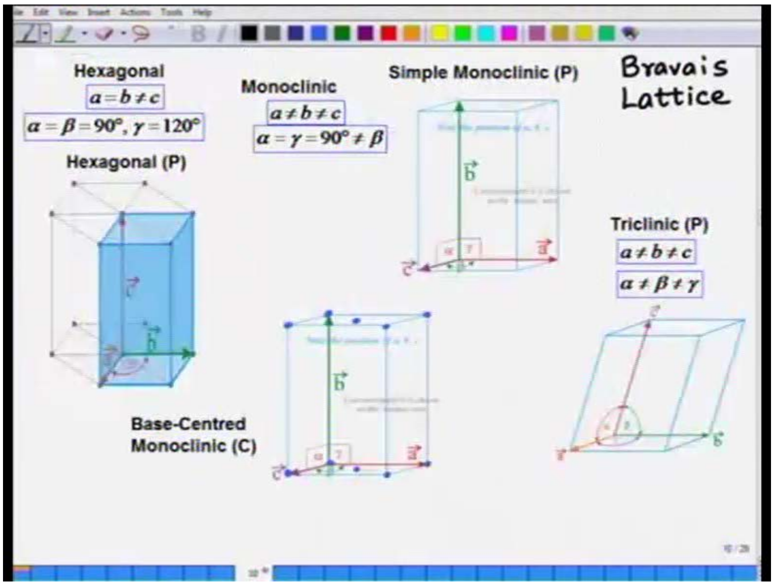

So, there is a cubic, tetragonal, orthorhombic, rhombohedral, hexagonal, monoclinic and triclinic depending… And, increasingly, cubic system has a highest degree of symmetry elements; and, triclinic has the least number of symmetry elements inherent in them. So, now, these unit cells – the way it works, is in 1848, there was a French crystallographer called – his name was Bravais – suggested based on the symmetry elements, they can only be precisely 14 point lattices. Based on the symmetrical combination of what we have looked at point, what is definition of point lattice; based on that definition of point lattice and the symmetry elements, which are underlying these point lattices, there can be exactly 14 Bravais lattices.

Those Bravais lattices have been drawn in this picture. And, you are quite familiar with it. Something is called (( )) There is a simple cubic. There is a body-centered cubic; there is a face-centered cubic; there is a simple tetragonal… There is a body-centered tetragonal; there is a simple orthorhombic – body centered orthorhombic, base-centered orthorhombic, face-centered orthorhombic, rhombohedral, hexagonal, simple monoclinic, base-centered monoclinic, triclinic. These are the 14 Bravais lattices, which I have drawn on this page here. So far, so good. And, up to here, I presume you all were very well-versed. Now, the point I want to make now is where things start; and, this is where you need to pay a little bit attention, because this is where we are going to be… It may become slightly confusing for you; that is where. So, just look at this. Let me do this; that if I take… There is no fundamental way; there is no requirement (( ))

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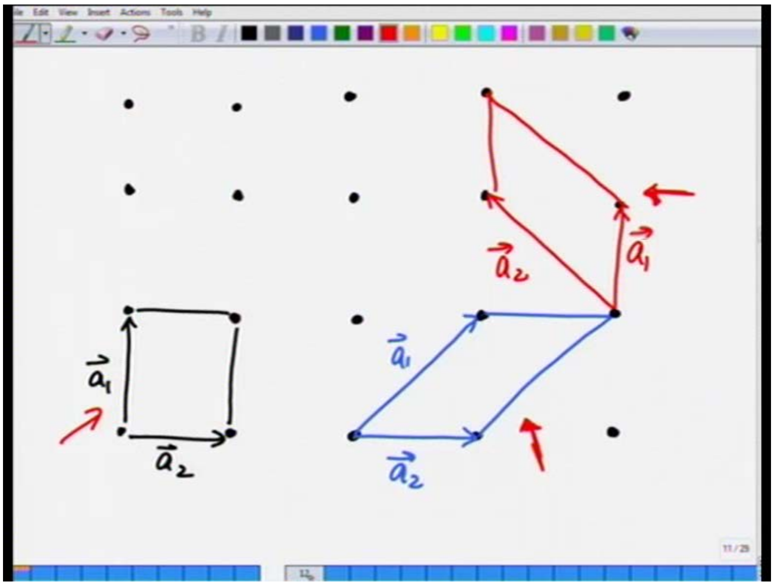

Let us take an example. Let us take an example like this in two-dimension again. The choice of unit cell is yours; how you choose your unit cell? For example, a person may choose a unit cell like this based on this a 1 and a 2 vector. And, you can always imagine the third one also in three-dimension. It is easier for me to draw in two-dimension. Another person may choose that, no, they might use this one as a 1 vector and this as a 2 vector, which will in this case define a volume area, which is like this; we will define an area, which is like this. Another person may choose something different in the sense that, exactly opposite they may choose this to be to the vectors a 1 and a 2. Let us say this is a 1; this is a 2; in which case, this structure will now look like… This unit cell will look something like this. All these are perfectly good unit cells; and, you notice their space filling; you translate them along directions of a 1 and a 2, multiples of integers; you translate them by… That means if you move by – change a 1 by integer or a 2 by integer, you will translate by that amount; then, you will fill the space and generate the lattice.

And, does not matter which unit cell you choose, there is no unique choice of these lattice vectors; you are free to choose the way you want to choose. Of course, there is a simpler way of choosing and there is a difficult way of choosing. Which is why you see normally, people choose like this; which shows the square symmetry of this lattice. Though this particular… This for example, This or this lattice has exactly same symmetry. But, for a person looking at it, it looks like a rhombus or a parallelogram; something like that it looks like. This unit cell look like parallelogram or a rhombus. They do not show symmetry of a square type lattice. Yes, it is not the square type; symmetry is not obvious; whereas, that underlying symmetry indeed does exist, because it is a same lattice after all. So, the choice of vectors you make is your choice. Sometimes, some choices will make things easier; sometimes they are difficult.

Nonetheless, let me now move on and try to explain another aspect, which is where what we will be interested in. And, next topic therefore, will be what is a… Next question would be what is a primitive cell? So, now, let us take this by example. Now, notice that, when we looked at cubic; if you looked at cubic; it came in three versions: simple cubic… Then, draw one more cube first. (( )) cubic lattice comes in three versions. Lattice points not atomic positions yet, no atoms, just imaginary lattice points here or here, here, here, here, here, here, here and one in the center or in these corners and also face centers.

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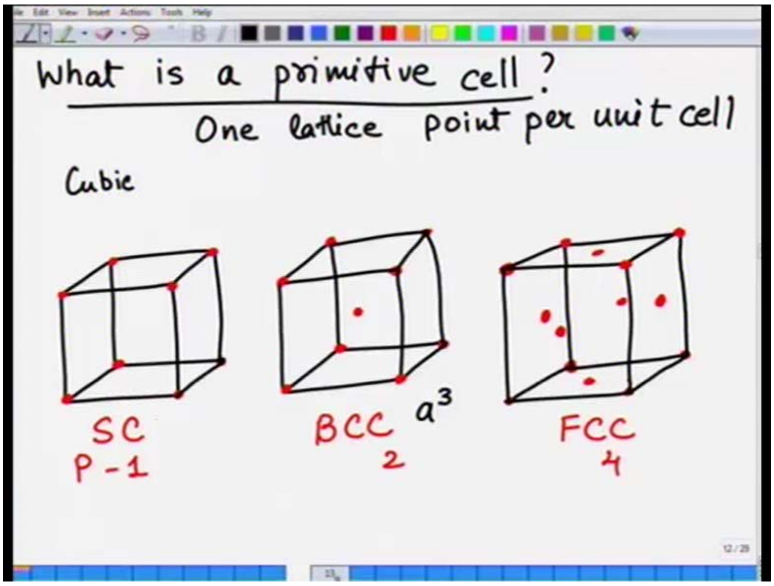

Now, on the front face. This is of course face centered cubic; this is body centered cubic; and, this is simple cubic. Notice that, how many lattice points we have per unit cell. In this cell, with lattice points only at the corners, I have one lattice point per cell; which means this… In this case, we call this as primitive cell. You will recall that. And then, there is a body centered has two; this has one point; this has two points per unit cell; and, this has four lattice points per unit cell. So, definition of primitive cell is one lattice point per unit cell. If you have one lattice point per unit cell, then it is called a primitive lattice. Clearly, simple cubic is the body centered cubic as shown; the unit cell shown is not a primitive unit cell. FCC has shown here is not a primitive cell, but it is always possible to make a primitive cell out of any structure. Now, if I have a BCC or I have a FCC, I still need a primitive cell. It is always possible to do so. And, I will show you by some example.

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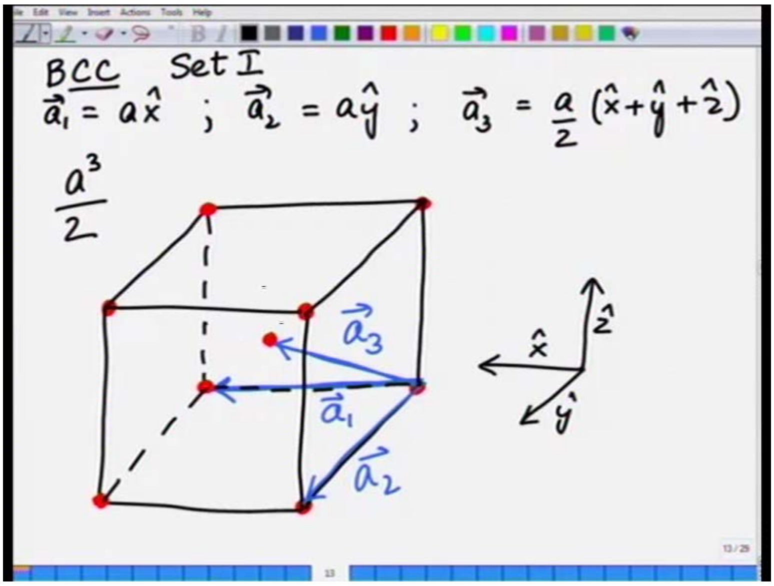

Let us assume… Consider BCC lattice. Let us choose vectors as a 1 as a x hat; a 2 as a y hat; a 3 as a by 2 – a being the lattice parameter, edge length of all these – x hat plus y hat plus z hat. Let us choose these lattice vectors. What does it look like? Let me draw it for you and then it might become little bit clearer for you. So, let us assume that it is something like this. Let us assume this cube to be like this. This is a BCC. Now, if you choose the lattice vectors as follows; you choose… You may choose another color now; use this as a 1. You choose this as a 1; you choose this as a 2; this is a 1. And, you choose one in the center. There is an atom in the center; you choose that as a 3 (( )). So, what I am going to do is I am going to draw an axis also. So, if you take an axis like this – x, y. So, this is the y-axis; this is the x direction and this is the z direction. Then, remember, what is the a 1? a 1 is a times in x direction. So, I am choosing this as a 1; this as a1. And, a2 is in y direction. So, I am choosing this as a 2. And then, third center point – body center point is selected as the a 3 vector, which is this vector.

Now, this is a 3. This is the a 3 vector. So, if I choose these vectors to be like this, now. you can notice that, whatever these three vectors generate, will be a volume, which will not look like a cube. But, it will be… Since the lattice point should be only at the corners of this vector; therefore, it will become a primitive vector – primitive unit cell, which will be defined by a 1, a 2 and a 3. If you wish, we can find the volume of this particular… through this enclosed by these vectors by taking the square product of it. And, you will find that, this volume is half the volume of a cube. If we take BCC like this, and the volume will here be a cube of course. And, if you calculate from here the scalar product, you will find the volume to be a cube by 2, because now, I have only one lattice point per unit volume. So, it will be half the volume only. Let me take another choice of lattice vectors. So, set 1. So, this is set 1.

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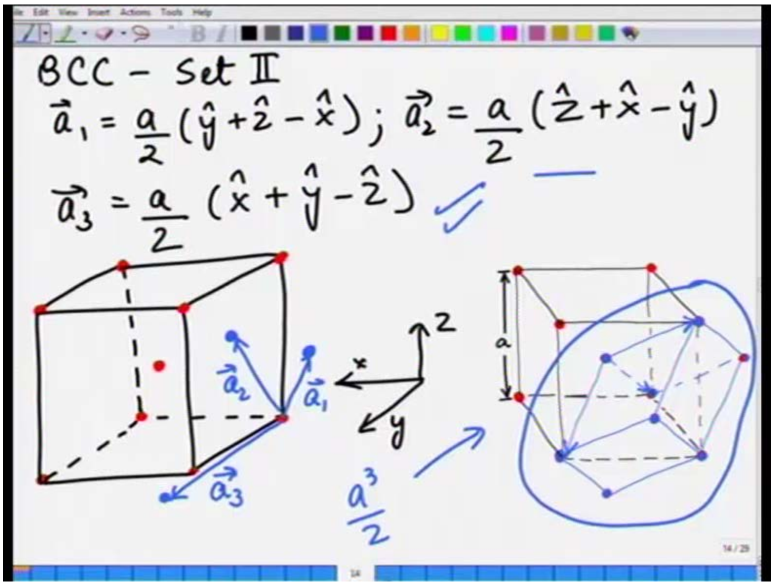

Let us take set 2. Let us say a 1 choose something like this – a by 2 y hat plus z hat minus x hat; a 2 as equal to a by 2 z hat plus x hat minus y hat; and, a 3 as vector a by 2 and x hat plus y hat minus z hat. Let suppose you choose vectors like this. You want to see this one; let me draw this also for you and show you how this one would look like; how these vectors would look like. Let us keep this big enough. I am trying to draw a cube though it does not look like exactly a cube. But, nonetheless, bear with me and use little bit of imagination also in here; only then it will probably work. So, I have a point here; I have a point here; I have a point here; I have a point here; point here, point here, point here, lattice point here; and, one lattice point of course, is there in the center also; there is a lattice point in the center also.

But, now, notice what I have done. This is what I have done is that, if you choose let us say let us choose an axis. So, this is x; this is x; this is y; and, this is z; this is z, going up z. Suppose this is the y direction; this is the y direction; this is the x direction and this is the z direction. This is how we are pursuing on this. So, if this is the case, let us draw this. How do these vectors look like? What you will find is remember, there are always going to be a point. There is another going to… There is going to be… Let me draw in blue ink probably. There is going to be another body centered point right here, which belongs to another unit cell, which comes out like this. There is another unit cell, which comes like this. Maybe this drawing is getting messy, messy, messy. So, we remove this – all these. And, I will leave this to your imagination actually. So, probably easier that way. So, let us do this.

Let us do it this way that, you imagine that, there is a unit cell right here; another unit cell which continues here. On this, you consider this face. And out of this face, out of this face, further, you see another unit cell. At the center of it, would be another lattice point. So, that lattice point I am going to draw right here. I am going to draw like that lattice point right here. Similarly, at this lattice point, when joined with this, you can see this vector a 1 vector; a1 vector; that means on the y and the z face center point; but, in x face in x-direction go negative direction. And, if you are in negative direction, that means you are coming out of this face and you will find a lattice point. Similarly, on a 2 vector, what you do is do the same thing; you look at the z and x face. z and x face and then you go out of that cell and out of cell z; and, over the face, which is formed by z, you will imagine this particular plane; this is the zx face, which is now given by z and x and minus y. In y-direction, you move half the distance in y direction. So, if you do that direction, then you will look at this point. Outside on this face are body-centered points.

Similarly, in this case, for a 3 vector, you see x and y plane – the bottom plain; you take the bottom plane and go down for the below. So, this will be the a 2 vector; this will be a 2 vector; and, going down, below will be a 3 vector. This is bad sort of… little bit bad drawing. But, if you draw this particular… Then, what you will have is you will have is now, you can imagine; if you wish another BCC cell; in this BCC cell, you can think like this – there is a lattice point, which has been taken. Now, if you… The unit cell will look much more like this. This is how the unit cell will look like – the shaded one. You can imagine this to be in context. Let us see if you have taken the center to be somewhere here, then you can go one out; this cell you can see unit cell, is in three directions coming out. And, this clearly does not look like a body-centered.

If you take these lattice vectors, then this is how you have to little bit do imagination; this is how the unit cell looks like. And, if the unit cell looks like this; and, its volume again will be half of what a cube is, because now, there are only going to be only one lattice point per unit cell. And, where are those lattice points? Those lattice points will only be at the corners. These are going to be the lattice points. And therefore, you can clearly see that, this is a primitive unit cell. So, it is always possible to make a primitive unit cell out of any… Whether it is BCC, FCC or any cell, it is always possible to make a primitive cell and there is no unique way of making primitive cell. For case of BCC, I have shown you two ways of making primitive cell. And, eventually, we will see, we will use this particular definition of lattice vectors for primitive cell. So, now, this BCC primitive cell as I have shown you, I mean, I have given you the set 2 vectors here – right here; and, I have shown you the structure of it. You please try drawing it yourself, because it does not quite look so nice. But, nonetheless, (( )) it is proper BCC cell; does not show BCC symmetry; which is why it is BCC always drawn some different way. But, it is always possible to make a primitive cell like this. And, these primitive cells are the ones which we use in analysis. So, these are the vectors, which we use. I promise in case of FCC, I will show you little bit better picture.

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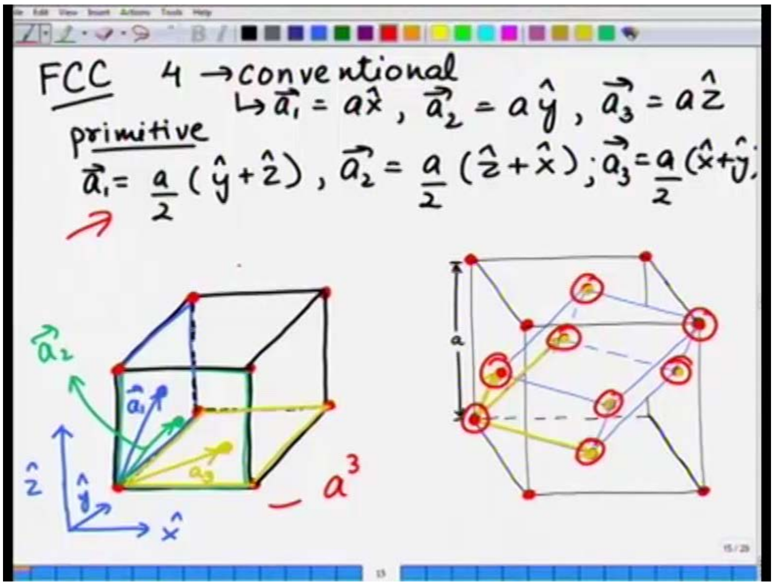

Let us use FCC. This is FCC. Now, you see FCC has four lattice points per unit cell. So, let us see how that looks like. Let me first give those lattice vectors to you. Let us say a 1 choice I make, one way is of course, you make a 1, a 2, a 3 as conventional. Conventional cell will have a 1 as a times x; a 2 as a y; and, a 3 as a z; which is same for BCC also. Just that there is a point at the face centers also in this case. And, you construct a unit cell using this; and, use that as a repeating unit; then, you can generate

FCC and you are having four lattice points per unit cell. But, primitive cell – let us construct a primitive cell. Let me show you how one can make a primitive cell from FCC also. By choosing, let us say I choose a 1 as equal to a by 2 y hat plus z hat; and, a 2 as equal to a by 2 z hat plus x hat; and, a 3 as equal to a by 2 x hat plus y hat. Choose the primitive cell like this.

Let me draw this for you this time it will be better. So, here I have shown you… I am going to move here and show you this unit cell first. So, here is an FCC unit cell, a cube; and, this red points, which you see here are the corner points. And, as we go along, I have shown you two FCCs and then I have shown you three FCC points: one blue, one green and one yellow. And, I am going to show you… And, I have not shown on this face; this particular face is the blue point. These three points, I have shown the face-centered points. But, I have not shown you face-centered points on other places just, so that the figure does not start looking bad. So, that is nonetheless you can imagine those points. So, let me move back here and let me draw these vectors for you. So, if I choose the orientation, if I choose the origin to be like this; so, if I choose the z to be like this – this direction; or, I will make it from here itself. So, I do it like this. z is this direction. And, this direction as I have drawn it in one direction here, one direction here; then, this is x direction and this is y direction and this is z direction.

Accordingly, let us see now, what a 1 is. If I look at a 1; so, a 1 will correspond to blue. So, if I take… a 1 is in y and z plane. So, I take this blue plane right here; this is the blue plane here; this particular plane and the phase center of it. Therefore, this is the a 1 vector. So, this is the a 1 vector. And, now, if I look at the a 2 vector, a 2 vector is in z and x plane. So, that is the one which will be given by this green stuff. So, let me draw the green one. So, if I consider this plane – this front plane; if I consider this front plane, then I can construct this vector. This is the face center point on this plane. This is a 2 vector. And similarly, if I take the bottom plan a 3, is an xy plane. So, if I take this one, then… So, the yellow plane. So, if I take this bottom plane right here; if I take this bottom plane and the face center point is right here; then, this is a 3; this is a 3.

Now, see what does it construct? What you get these three… If I choose these three vectors, what do I get? What you can get now is I am showing you these three vectors as… These are the three vectors right here: this one, this one and this one are those three vectors. If you have these are the three vectors and you construct a volume out of it; then, you get a nice structure like this, which is shown here. And, you can see that, this is a primitive cell with lattice points right here, right here, right here, right here, right here, right here, right here, right here. Of course, these two… Let me use another pen; this point and this point are the two corner points of this FCC lattice, which may be marked in red; I mark them in this red. Rest of the points are all face-centered points; rest of the points are all face-centered points. At this on the top, the face-center point on the bottom; here is a face center on the front; here is a face center point on the back; here is a face center on the right; here is a face-center point on the left. So, here are the face-centered points.

Now, if you calculate the volume of this cell, it will be exactly one-fourth of a cube; a cube was the conventional cell, which will be the volume of… Whole cube had a volume of a cube. But, since this is… And, that would have four lattice points per unit volume; if you now calculate using the scalar product of these three vectors, you calculate the volume; you will get one-fourth of the volume. But, this is nice primitive cell.

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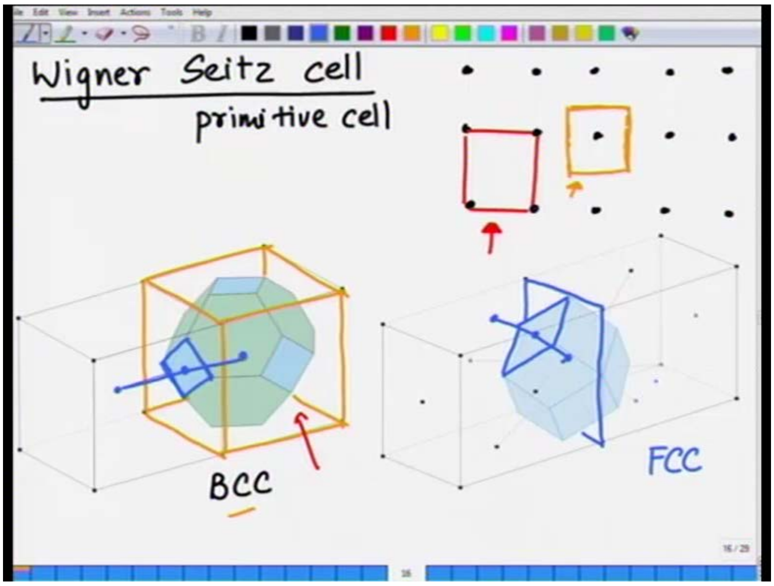

Before I end on the subject on primitive cell, I will show you another kind of primitive cell, which is called as Wigner Seitz cell. So, last topic in this crystal structures is this Wigner Seitz cell. Another way of making a primitive lattice is as follows. Take for example, this BCC. Take this as primitive cell. This is also a primitive cell. Let me first make it into two-dimension maybe to show you to make the point. Suppose I take a square lattice in two-dimension like this. And, instead of choosing a primitive lattice like this, primitive unit cell in two-dimension like this, which I could. Another way to choose this will be like this. And, this particular cell, which I have shown you in red right here has one lattice point per cell, because lattice points are only in the corner. If I take this one, I can choose… Another way of choosing a lattice point is like this if I choose my unit cell to be like this. If I choose the unit cell to be like this, notice – this also has only one lattice point.

Now, the lattice points are not at the corner. But, this is also repeating unit. If I repeat this unit, I generate the hole. This is also a good unit cell. There is only lattice point is in the center; there is no lattice point. And, this is only… This is also a primitive unit cell, because it has one lattice point per unit cell. Exactly, same thing can be done for different crystal structures. For example, take this BCC example. Imagine this to be one cube; here is one cube. Take this one cube here – right here. Take this one particular cube here. Draw… Take this one cube. Now, you know that, you have one lattice point right in the center. From that center, draw lines to all other lattice points; take perpendicular bisectors of them. And, what is left then is this kind of structure, which is shown here.

You take perpendicular bisectors and find what is the smallest volume. So, from the center point, you draw lines to all other lattice points – all the lattice points; draw planes, which are perpendicular to these lines right in the center of two… Whatever the line is joining two lattice points, right in the center of it or center of this line, draw a perpendicular plane. Keep drawing it like this. For all the lines, you can possibly draw and construct the smallest volume. In case of BCC, clearly, as the geometry shows you that, if I have a center… Let us take an example. I have a center point; I have a center point. Here is this line. And, this is the perpendicular bisector for it. This is the plane, which is perpendicular bisector for it; which intersects at this particular point here. And then, I make this smallest volume like this. Then, what you have is a primitive cell, because the only thing which is in there is one point in the center. And, that is called a Wigner Seitz cell.

Similarly, it is done here for FCC. You can now imagine that, on this face conventional cell, this is one of the face of the cube. On this face, right in the center will be a face-centered point. From this face-centered point, you draw perpendicular bisectors to all other points, which are there. For example, you draw from here a perpendicular bisector to the top phase like this and it intersects here. And, construct this plane. And, on this plane, it intersects right here. And, in this way, you construct this particular volume. This is also Wigner Seitz cell. Right in the center is a lattice point. Why am I talking about this particular cell? Because this will become an interesting point. This is precisely the kind of cell we will be looking for in reciprocal lattice. So, with this, I would like to close the chapter on this crystal structures or lattices.

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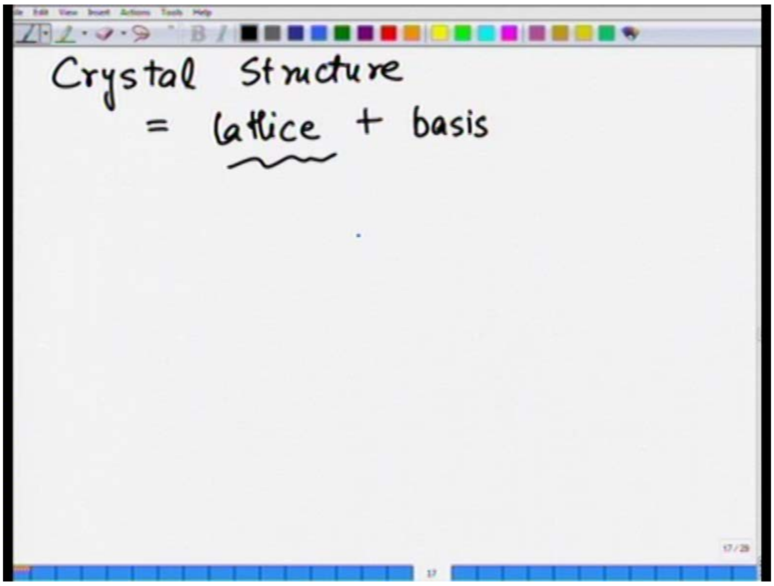

But, last point, maybe should I say what is crystal structure, because I have not said crystal structure. That I will not go through, but crystal structure is simply lattice plus a basis; that means on all the lattice points, which you have, you start putting now atoms; and, whatever the basis is – one single atom, two atoms, multiple atoms – whichever you want to put it, that generates a crystal structure. And, I will advise you that, please brush up your knowledge on this crystal structures and also brush up a little bit on the directions and planes in this crystal structures, which we will frequently use and maybe useful.

But, in the summary, what we want to do is in summary, there is a point lattice; there is an underlying symmetry in the point lattice. Based on that, there are exactly fourteen Bravais lattices possible. Some are primitive, some are not primitive; whichever are not primitive, it is always possible to make a primitive lattice. Primitive lattice has one lattice point per unit cell. And, primitive lattices are often used in analysis, which we will do. Shown here is for BCC; then, shown here is for FCC – a primitive lattice. But, there is another construct for primitive cell, which is a Wigner Seitz cell. This Wigner Seitz cell here may not be too much of importance at least for us. But, this will become same construction in reciprocal space, would become lot more important.

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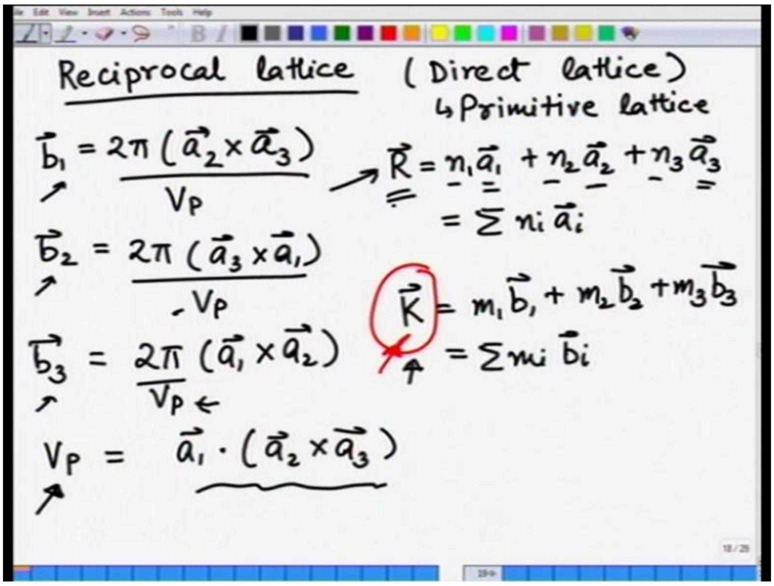

So, this is where I would like to finish the topic of crystal structures and move onto what is called as reciprocal lattice now. I introduce this topic and then finish in the next lecture. So, here is reciprocal lattice. Let us start with this. So, now, notice a direct lattice. We will use the word direct lattice; in contrast, we have a direct lattice. What we just did was direct lattice. So, for this direct lattice, I will write a lattice vector R, which is… We will use the symbol n 1 a 1 plus n 2 a 2 plus n 3 a 3. And, I will always use a primitive lattice; which means… Let us go back for BCC for… Let us go back and look at this BCC; that means I am going to use a 1, a 2 and a 3 like here. I will choose a 1, a 2, a 3.

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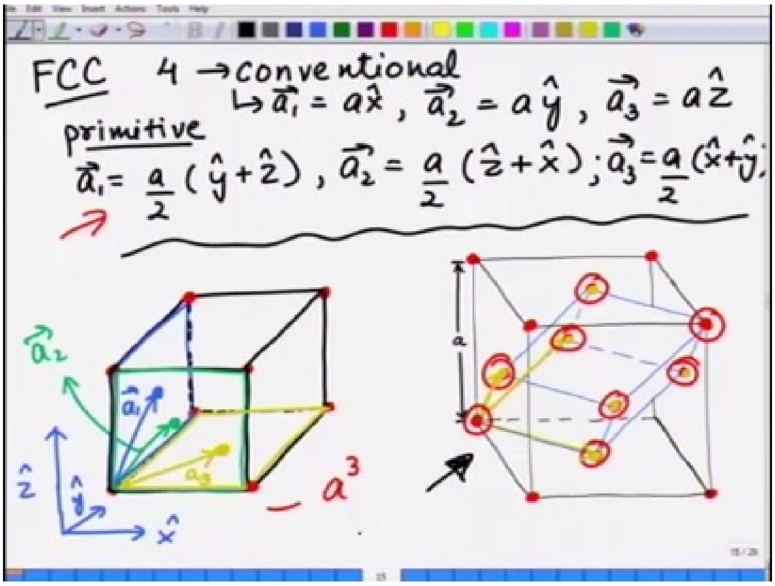

Similarly, if I take in FCC, I will choose the lattice vectors a 1, a 2, a 3 to be like this. If I choose the lattice vectors in this fashion, I generate this structure. And remember, in this case, if I generate, if I change n 1, n 2 and n 3 like I am drawing here. If I choose values of n 1, n 2, n 3 – all integer values of n 1, n 2 and n 3. With this choice of a 1, a 2 and a 3; since this is primitive, because the points lie only on the corners of the unit cell. Therefore, by choosing n 1, n 2 and n 3, this is a lattice vector by which I can generate all the lattice points by choosing n 1, n 2, n 3. If I choose n 1, n 2, n 3 as zero – all zero, then I will start with some point, that is, the lattice point. And then, I keep choosing n 1 equal to 1, n 2 – 0; n three – I will get another lattice point. And, I will keep doing… If it is not primitive cell, then you will not be able to generate all the lattice points by choosing n 1, n 2 and n 3 as integers. But, because it is a primitive cell, then R is truly a lattice vector, which will generate all the lattice points.

Now, similarly, I am going to do is I am going to just write some vectors now. First, I am going to do is this. I am going to write b 1 vector, which I am going to write 2pi multiplied by cross product of a 2 and a 3 divided by a volume of… I will show you what volume of a primitive cell of this primitive cell. I will write b 2 vector; just do not worry; just think that, there is something being written. What it is? We will see what it is. a 3 into a 1 cross product divided by same V p. And, I will write b 3 as equal to 2pi by V p volume of this a 1 cross a 2. I am just going to write it like this. And, I am going to construct a vector called k – this vector as m 1 b 1 plus m 2 b 2 plus m 3 b 3. In fact, let me write this as simply as n i a i and this as therefore, m i b i, where i of course, is 1, 2, 3. i is 1, 2, 3 only. So, this is k vector I am writing. And, V p in this case is… And, the V p is just the scalar product a 1 dot a 2 cross a 3. This is a scalar product, which gives me the volume of the primitive cell. So, if I ask what is a primitive cell constructed by; I construct a primitive cell with this vector; a 1, a 2, a 3 are vectors which construct the primitive cell. One wants to know what is the volume of the primitive cell in the direct lattice. Then, the volume is just simply this quantity V p – the volume of the primitive cell. So, I have divided this by volume of primitive cell. And then, I generate a vector called K based on this; where, m 1, m 2, m 3 now are integers. What happens and why are we doing this is basically the story. What it means?

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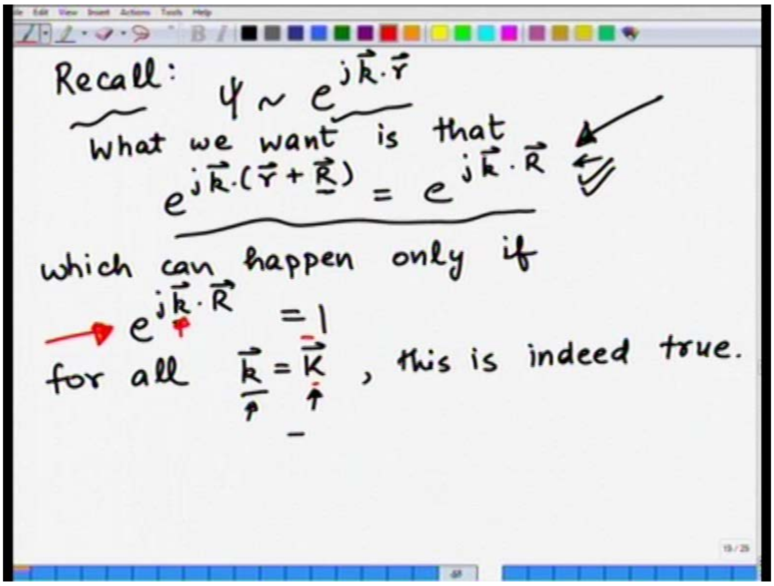

Recall – our wave function had a form of e to power j k dot r. That is the form. Recall wave function, which we had derived in free electron theory had this form. And also, this is a plane wave form essentially. Now, what we want is that phi of r (( )) What we want is that, e to the power j k r – dot product – r plus R should become equal to e to power j k dot r. Why? See this represents the periodicity of the lattice that, in the lattice, if you move by this vector R, then you essentially add the same point. This is the definition of point lattice, remember. So, if you move from one point to another point by this translation vector R, then the lattice looks identical; there is no difference in it. So, we want… And, since we are going to deal with properties in this kind of lattice, then since these points are not different, they are identical; then, the behavior of anything should also look similar. So, if the wave function has this form, then it should also acquire same character at those some special points. So, this is why we want that this to happen, because that we want that, there should be periodicity of R in wave function also, which can happen only if you can see that; that means e to the power j k dot R should be equal to 1; small k I have drawn; small k dot R should be equal to 1. If this happens, then this will be true; then, this particular thing will be true in there.

Now, notice for all k's, which are like the capital K, which we have just derived; here is a capital K, which we have just derived. And, this capital K, which we have just derived – if we substitute this particular capital K for all small k's in here equal to this capital K, this is indeed true. So, that is what essentially we would like to do here that, if you for some special values of k; k remember is a reciprocal space. Now, if you look at the dimension of this quantity b 1, b 2 and b 3; then, it is also inverse of length. Remember a2 cross a3 divided by a volume. Therefore, that is also an inverse of length. So, k clearly – small k clearly… This capital K vector clearly belongs to a reciprocal space as do the… This small k vector indeed belongs to a… Small k vector – we know it belongs to the reciprocal space; and, so does capital K. If these two become equal, then this relationship, which is shown here becomes true. So, this is the reason why we have generated this k vector in a form as we have.

And, you please try that. You substitute in here. In this expression, substitute this capital K here and see indeed if it gets one or not by choosing b 1, b 2, b 3 as we have. That is a small part of the story. But, if you are familiar with this, you can see that, if this is true in the plain waves, I can form a complete set; I can do a fourier analysis. And, for all periodic functions, we would be able to do fourier analysis. Any function, which has periodicity of capital R, then I would… In this case, this is only good set to do fourier analysis. That is essentially what it means. But, I will not… And, that is what we do for x-ray diffractions, etcetera. But, in this course, we will not go through it; we will just… Since my intention is to show you what is consequence, how to represent E-k diagram, so, I will limit my discussion only to that. We will continue on this part… Since now, I have constructed b 1, b 2, b 3 as vectors just like a 1, a 2, a 3, a 1, a 2, a 3 construct… From a 1, a 2, a 3, we could construct a primitive lattice. Similarly, with b 1, b 2, b 3, these vectors in reciprocal space, we should be able to construct another set of lattice in reciprocal lattice. And, those we will call as reciprocal lattice constructed by b 1, b 2, b 3, which we will start in the next lecture.

Thank you.